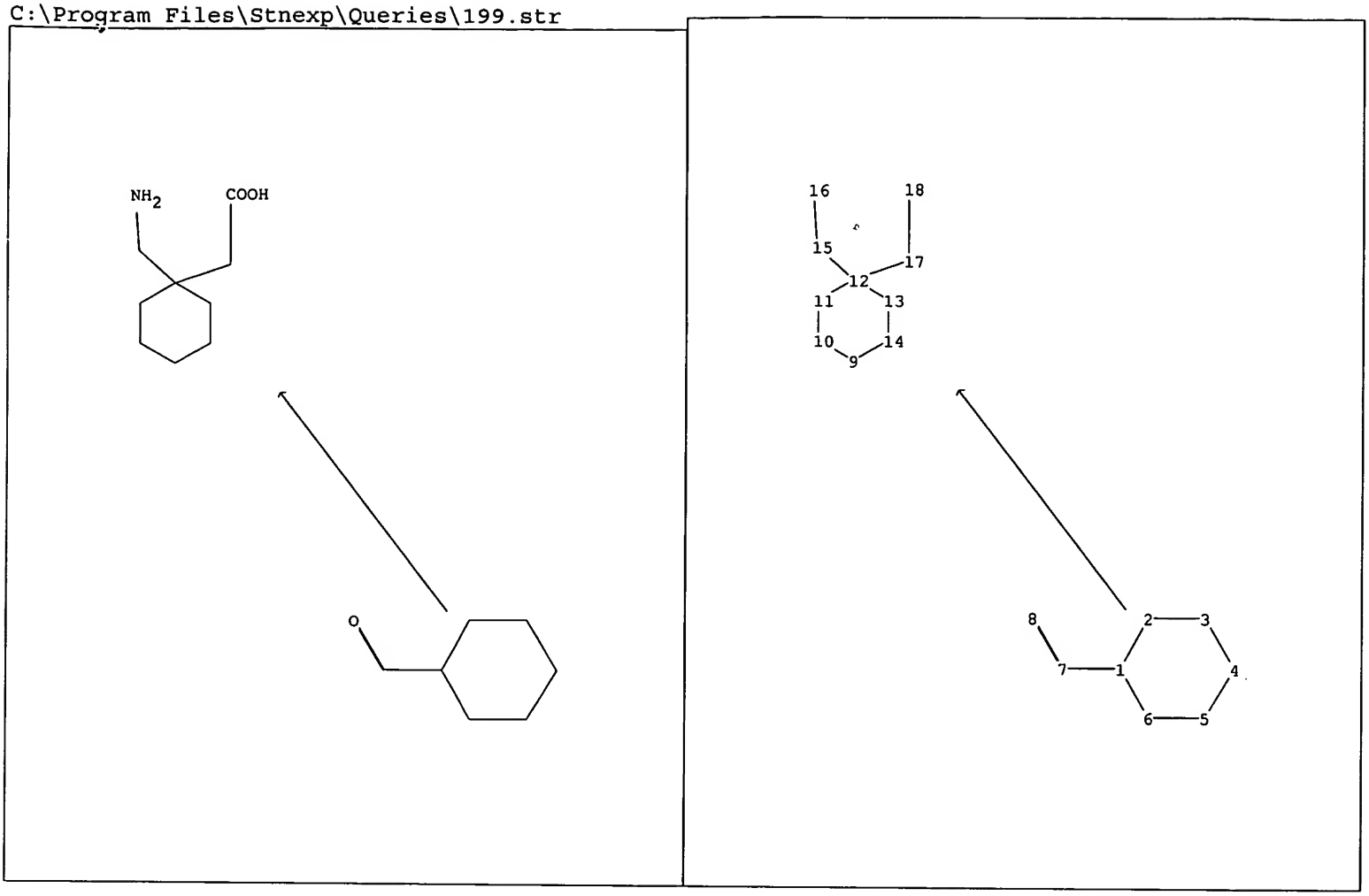
C:\Program Files\Stnexp\Queries\199.str



chain nodes :
15 16 17 18
ring nodes :
1 2 3 4 5 6 9 10 11 12 13 14
ring/chain nodes :
7 8
chain bonds :
12-15 12-17 15-16 17-18
ring/chain bonds :
1-7 7-8
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14
exact/norm bonds :
1-7 9-10 9-14 10-11 11-12 12-13 13-14 15-16
exact bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 12-15 12-17 17-18

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS
fragments assigned product role:
containing 9
fragments assigned reactant/reagent role:
containing 1

0 SEA SSS SAM L1 (0 REACTIONS)

=> s l1 sss full
FULL SEARCH INITIATED 16:06:34 FILE 'CASREACT'
SCREENING COMPLETE - 856 REACTIONS TO VERIFY FROM 67 DOCUMENTS

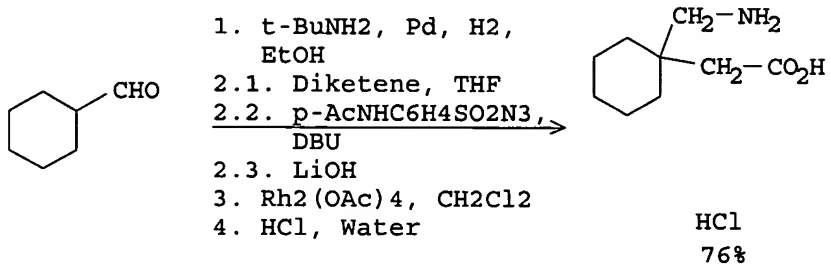
100.0% DONE 856 VERIFIED 20 HIT RXNS 5 DOCS
SEARCH TIME: 00.00.01

L3 5 SEA SSS FUL L1 (20 REACTIONS)

=> d 1-5

L3 ANSWER 1 OF 5 CASREACT COPYRIGHT 2006 ACS on STN

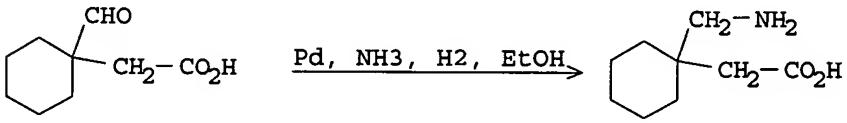
RX(24) OF 30 - 4 STEPS



REF: Faming Zhuanli Shenqing Gongkai Shuomingshu, 1541995, 03 Nov 2004
CON: STEP(1.1) 12 hours, 50 deg C, 1 atm
STEP(2.1) 0 deg C; 0.5 hours, 0 deg C; 8 hours, 0 deg C -> room temperature
STEP(2.2) 12 hours, room temperature
STEP(2.3) 8 hours, room temperature
STEP(3.1) 3 hours, reflux; 2 hours, reflux
STEP(4) 12 hours, reflux

L3 ANSWER 2 OF 5 CASREACT COPYRIGHT 2006 ACS on STN

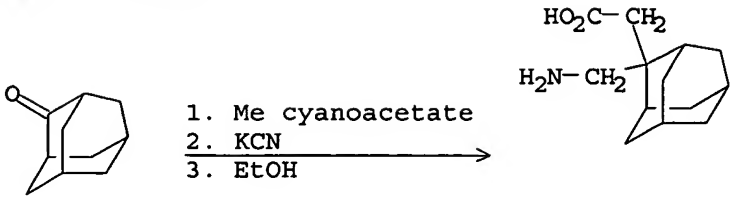
RX(1) OF 37



REF: U.S. Pat. Appl. Publ., 2005148792, 07 Jul 2005
NOTE: green chemistry, palladium supported on carbon is used as catalyst
CON: STAGE(1) room temperature; 4 hours, room temperature, 50 psi

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2006 ACS on STN

RX(26) OF 26 - 6 STEPS

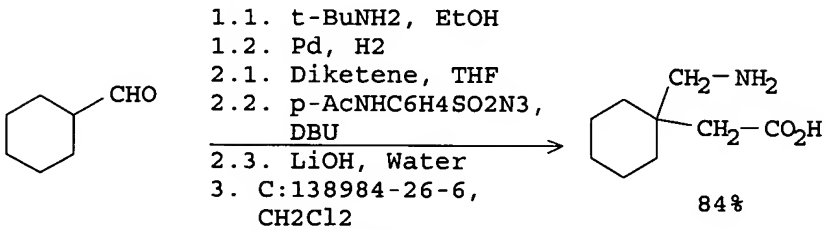


HCl
80%

REF: Bioorganic & Medicinal Chemistry, 13(8), 2791-2798; 2005
NOTE: 3) key intermediate(in synthesis of GABA adamantane derivative), 4) alternate preparation also described, 5) alternate preparation also described
CON: STEP(1) 6 hours, reflux
STEP(2.1) 25 hours, reflux
STEP(3.1) <room temperature; 20 days, room temperature
STEP(4.1) 24 hours, 20 deg C
STEP(5.1) 48 hours, room temperature
STEP(5.2) <room temperature, acidify
STEP(6) 5 hours, 25 deg C, 50 psi

L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2006 ACS on STN

RX(69) OF 73 - 4 STEPS

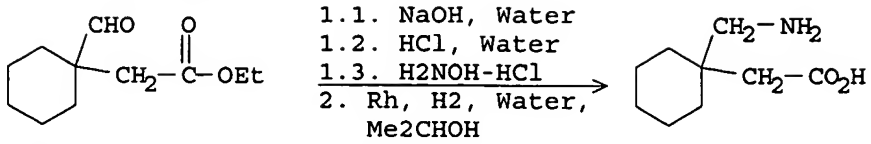


84%

REF: Tetrahedron, 61(6), 1579-1586; 2005
NOTE: 3) optimization study, regioselective, optimized on catalyst and catalyst concentration
CON: STEP(1.1) 1 hour, room temperature
STEP(1.2) 12 hours, 50 deg C, 1 atm
STEP(2.1) 0.5 hours, 0 deg C; 0 deg C -> room temperature; overnight, room temperature
STEP(2.2) 8 hours, room temperature
STEP(2.3) 8 hours, room temperature
STEP(3.1) 2 hours, reflux; 30 minutes, reflux
STEP(4) 18 hours, 90 - 120 deg C

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2006 ACS on STN

RX(5) OF 6 - 2 STEPS



REF: PCT Int. Appl., 2002074727, 26 Sep 2002

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